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INVERSION OF EXPERIMENTAL OPTICAL DATA

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Contract No. DAAK11-82-C-0104

February 1984

US Army Armament, Munitions & Chemical Command Aberdeen Proving Ground, Maryland 21010

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REPORT DOCUMENTATION PAGE	READ INSTRUCTIONS BEFORE COMPLETING FORM			
	3. RECIPIENT'S CATALOG NUMBER			
CRDC-CR-84018 AD- ALS	979			
4. TITLE (and Subtitio)	5. TYPE OF REPORT & PERIOD COVERED			
INVERSION OF EXPERIMENTAL ORTICAL DATA	Contractor Report			
INVERSION OF EXPERIMENTAL OPTICAL DATA	13 Aug 82 - 13 Sep 83			
	6. PERFORMING ORG. REPORT NUMBER			
7. AUTHOR(a)	8. CONTRACT OR GRANT NUMBER(*)			
C. D. Capps				
A. R. Tokuda G. M. Hess	DAAK11-82-C-0104			
9. PERFORMING ORGANIZATION NAME AND ADDRESS	10 PROGRAM EL EMENT PROJECT TASK			
Boeing Aerospace Company	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS			
PO Box 3999				
Seattle, Washington 98124				
11. CONTROLLING OFFICE NAME AND ADDRESS	12. REPORT DATE			
Commander, Chemical Research and Development Center				
ATTN: DRSMC-CLJ-IR (A)	13. NUMBER OF PAGES			
Aberdeen Proving Ground, Maryland 21010 14. MONITORING AGENCY NAME & ADDRESS(II different from Controlling Office)	47			
Commander, Chemical Research and Development Center	, , ,			
ATTN: DRSMC-CLB-PS (A)	UNCLASSIFIED			
Aberdeen Proving Ground, Maryland 21010	154. DECLASSIFICATION/DOWNGRADING SCHEDULE			
NA 16. DISTRIBUTION STATEMENT (of this Report)				
Approved for public release; distribution is unlimited.				
17. DISTRIBUTION STATEMENT (of the abetract entered in Block 20, If different from Report)				
18. SUPPLEMENTARY NOTES				
Contracting Officer's Representative: Dr. Bottiger (DRSMC-CLB-PS (A)) (301) 671-2395				
19. KEY WORDS (Continue on reverse side if necessary and identify by block number)				
Inversion Remote Sensing Analytic Inversion Constraints and Inversion				
20. ABSTRACT (Continue on reverse side if necessary and identify by block number)				
Particle size distributions were obtained by inversion of simulated scattering data using an analytic algorithm. An extension of the analytic inversion technique to incorporate constraints is also presented.				

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PREFACE

The work described in this report was done under Contract No. DAAK11-82-C-0104. This work was started in August 1982 and completed in September 1983.

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INVERSION OF EXPERIMENTAL OPTICAL DATA

1. \ INTRODUCTION

There exist several inversion techniques for inferring the particle size distributions from scattering measurements done on aerosols composed of spherical particles. This report will treat several areas related to the practical application of inversion algorithms to actual experimental measurements to obtain size distributions.

The first area to be discussed is the one of which measurements to make. Due to the nature of the Mie function which describes the scattering process certain measurements contain more information than others. However, practical considerations, e.g., availability of sources, optics, and detectors, limit what experiments can be done. Optimization of the measurement process under both of these constraints will be discussed in Section 2.

Section 3 presents the data that will be used in the inversion and preliminary analysis. In order to invert the data it is necessary to first estimate the radius range spanned by the particles in the distribution. This is done by fitting the data with a log-normal size distribution and inferring the radius range from the fitted parameters.

In Section 4 an analytic inversion technique will be applied to the simulated experimental data provided by the Chemical Research and Development Center (CRDC) to obtain particle size distributions. This analytic method was developed to provide a better understanding of the inversion process, i.e., how the information content of the measurement set influences the uncertainty in the calculated size distribution. As this was a blind test, i.e. the size distributions were unknown to those doing the inversion, the insights achieved with this method are especially relevant to the practical inversion problem.

Section 5 will discuss an extension of the analytic inversion method in which constraints can be added to improve the inversion and yet

the effects of the data and constraints can be separated quantitatively. Recommendations for future research are made in Section 6.

OPTIMIZATION

The technique used to select the optimal measurement set has been described in detail.1,2 Briefly, the method involves determining the number of independent pieces of information contained in a large set of possible measurements through the use of an eigenanalysis of the measurement covariance matrix. Superfluous measurements are excluded one at a time according to the algorithm until the number of measurements and independent pieces of information are approximately equal. The measurement set with the largest number of independent pieces of information is taken as the optimum as it contains the most information about the range of particle sizes.

Basically, three types of mesurements were examined for particles in the range 0.002 to 2.6 microns in diameter. These were intensity in the backscatter direction at different wavelengths, intensity at one wavelength over a range of scattering angles in the near forward direction, and polarization at one wavelength over the full range of scattering angles. The optimal set was found to be wavelength dependence of the intensity in the backscatter direction. These wavelengths are listed in Table 1.

Table 1. Optimal Wavelength Set

Kerne l	Index Wave	length (microns)
1		0.266
2		0.524
3		0.782
4		1.04
5		1.55
6		2.33
7		2.59
. 8		2.85
ğ		3.63
10		3.88
11		4.14
12		4.91
12		

It must be recognized that this set is based on a limited search. The search region should be broadened considerably in order to confidently establish an optimum measurement set.

Two explicit suggestions can be made in regard to this search; the wavelength of 0.266 micron is not practical for field measurements and should not be included in a real set, and the range of particles sizes should be increased so that the upper limit on diameter is approximately 10 microns. Futher recommendations will be made in Section 6.

3. PRELIMINARY DATA ANALYSIS

The system modeled for this simulated experiment was a paydisperse hydrosol of polystyrene latex spheres. Five distribution functions known only to the Chemical Research and Development Center, were used created the five synthetic data sets labeled by the letters "A" through "E". These sets were created by multiplying a distribution function by the total and differential cross sections given by Mie theory for 15 different wavelengths and integrating over particle radius. In order to simulate actual experiments a random error with a known variance was added to each data item. Each of the five data sets then consisted of the total and differential cross sections at 15 wavelengths with the error included. Table 2 lists the wavelengths in the water medium and the latex/water relative refractive indices used.

Table 2. Optical Parameters

Wavelength in Water	Relative Refractive
(microns)	Index
0.222	1.2563
0.266	1.2275
0.524	1.1900
0.782	1.1861
1.04	1.1889
1.55	1.2017
2.33	1.3397
2.59	1.1330
2.85	1.1529
3.63	1.1779
3.88	1.1859
4.14	1.2005
4.91	1.1725
6.20	1.2133
8.99	1.3286

As discussed in Section 2 the optimum measurements are the backscatter cross sections at the wavelengths given in Table 1. These are included in the CRDC data sets. Therefore, the inversion work presented in this report will use the backscatter cross sections listed in Table 3 as its basic data.

Table 3. Backscatter Cross Section (Micron²)

Wavelength	Set A	Set B	Set C	Set D	Set E
0.222	9.13	9.95	4.01	15.7	3.08
0.266	12.6	15.9	5.78	19.0	2.68
0.524	6.27	6.66	8.36	26.0	1.81
0.782	1.72	1.68	4.75	8.93	.602
1.04	.831	.856	2.42	4.24	.294
1.55	.463	.555	.924	1.69	.179
2.33	2.10	2.61	2.69	4.88	.490
2.59	.109	.143	.0788	.182	.0292
2.85	.168	.194	.101	.295	.0417
3.63	.242	.344	.117	.529	.0645
3.88	.262	.361	.142	.626	.0711
4.14	.319	.444	.182	.822	.0863
4.91	.184	.195	.126	.475	.0541
6.20	.260	.300	.257	.752	.0751
8.99	.554	.644	.507	1.39	.119
Fractional Error	.03	.10	.03	.03	.03

The first step in the analysis of the data is to determine the size range of the particles present in the distribution. This is necessary for In order to numerically integrate over the rapidly oscillating Mie cross section it is necessary to have a large number of integration points per radius interval; approximately 400 points per micron for 0.10% accuracy for the wavelengths listed in Table 3. Computation time is, therefore, significantly increased if a larger than required radius interval is used. Secondly, the backscatter cross section is essentially the product of a function that oscillates about an equilibrium value and the radius squared. If larger radii than needed are included sensitivity to the smaller, significant radius values is reduced. This is easily seen in Figure 3 of the second literature cited. The portion of the distribution function that is recoverable by inversion is a linear combination of functions of the form plotted in that figure. As none of the functions shown have significant values for radii less than about 0.4 microns it would be impossible to construct a distribution function that had its major contribution in this region. Thus, it is important both for theoretical and practical reasons to bound the radius region before an inversion is done.

This was accomplished by first fitting the data with a log-normal particle size distribution which has the form

$$f(r) = \frac{N}{r \ln s 2\pi} \exp \left(-\frac{1}{2} \left(\frac{\ln 2r - \ln D}{\ln s}\right)^2\right)$$
 (1)

where N = total number of particles

D = geometric mean diameter

s = geometric standard deviation.

The rationale for this function is that it is found in many natural particle size distributions involving condensation phenomena and that it is significant in only a limited region. The predicted backscatter cross section σ_p (λ , N, D, s) is given by

$$\sigma_{\rm p}$$
 (λ , N, D, s) = $\int_0^5 \sigma_{\rm m}$ (r, λ) f(r) dr (2)

where λ = wavelength

om = Mie theory backscatter cross section.

The upper limit of 5 microns in the integral was provided by CRDC. In a real problem this upper limit would have to be determined by physical considerations, such as settling rates. The parameters N, D, and s were estimated by using a Marquardt-Levenberg³ algorithm to minimize chi-square for each data set. Chi-square is defined as

$$\chi^2 = \sum_{\lambda} \left(\frac{\sigma(\lambda) - \sigma_p(\lambda)}{e \ \sigma(\lambda)} \right)^2$$

where $\sigma(\lambda)$ are the backscatter cross sections and c is the fractional uncertainty listed in Table 3. The resulting parameter values are given in Table 4 and the corresponding plots of f(r) in Figures 1-5.

Table 4. Values From Log-Normal Fit

Set	Number of <u>Particles</u>	Geometric Mean Diameter (Micron)	Geometric Standard Derivation
Α	0.829	2.85	1.40
В	0.959	3.03	1.33
С	0.579	1.61	5.56
D	0.745	4.33	1.36
E	1.03	0.952	2.07

Even if the actual distribution is not a log-normal the above fitting procedure should produce useful information about the range of particle sizes. For example, if the actual size distribution were bimodal the fit could place the single log-normal peak at an intermediate position and increase the width to include the significant portion of the distribution. The radius range used in the inversion was the region that included 99% of

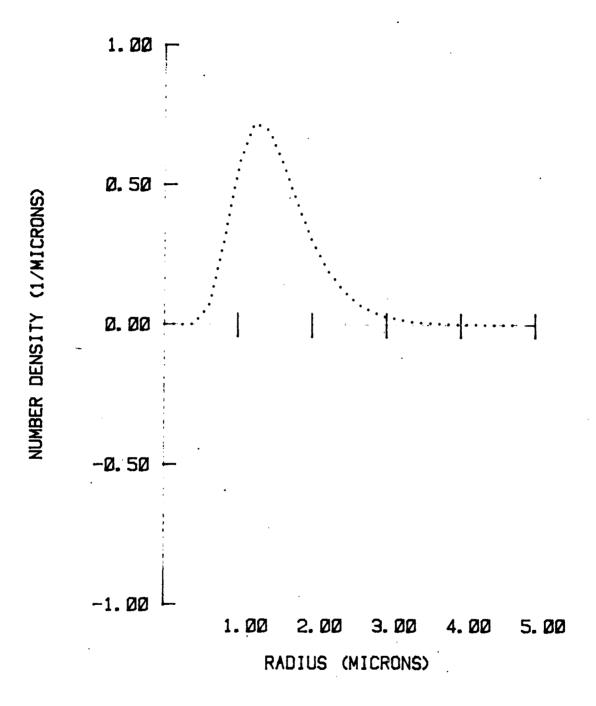
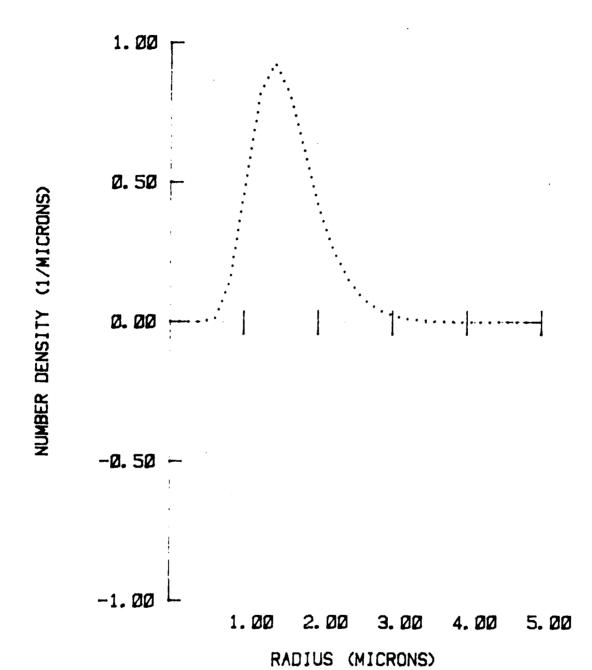


Figure 1. Log-normal Size Distribution Fit to Set A



2. Log-normal Size Distribution Fit to Set B

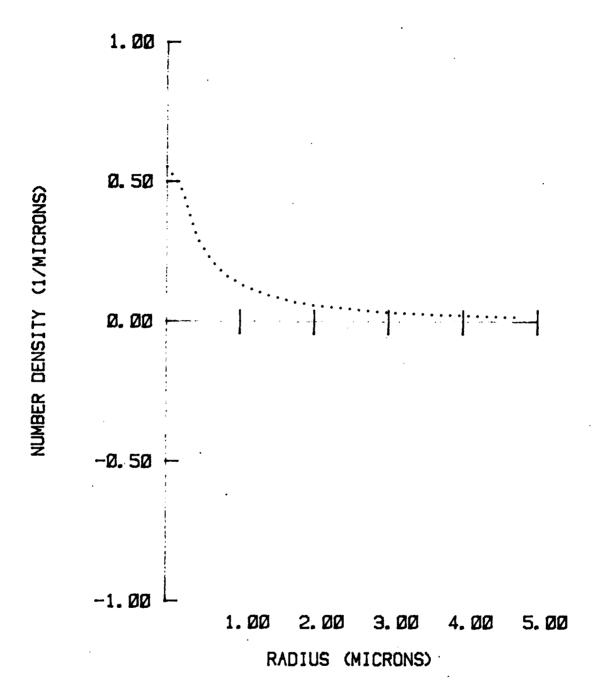


Figure 3. Log-normal Size Distribution Fit to Set C

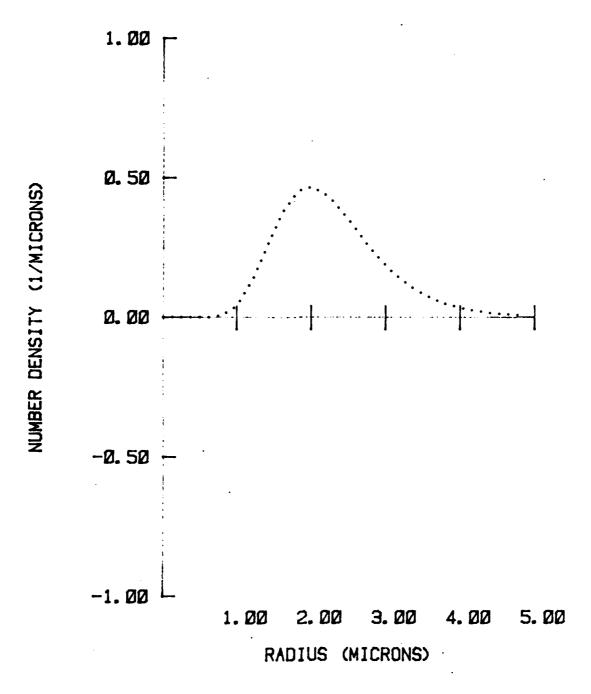


Figure 4. Log-normal Size Distribution Fit to Set ${\tt D}$

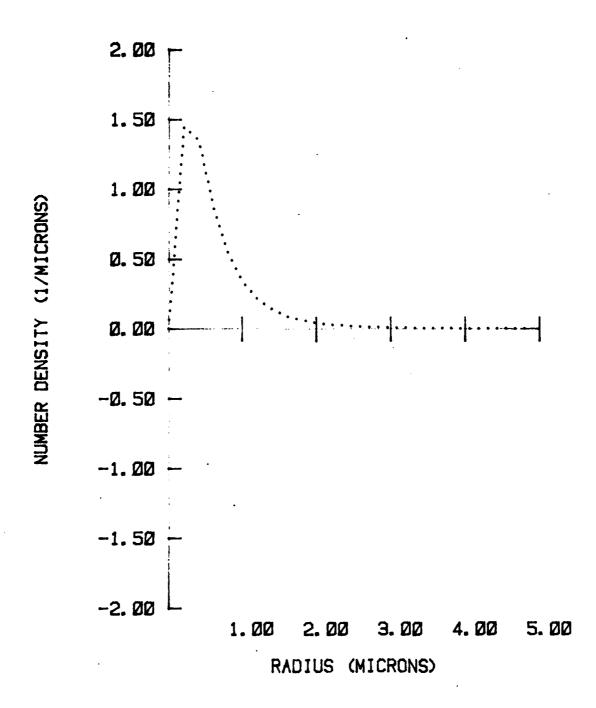


Figure 5. Log-normal Size Distribution Fit to Set E

the area under the distribution f(r). The upper and lower limits on r are calculated from the fit parameters D and s

$$r \pm \frac{1}{2} (\frac{0}{2}) s^{\pm 2.6}$$
 (4)

and are listed in Table 5.

Table 5. Radius Region Used for Inversion

Set	Minimum Radius (Microns)	Maxium Radius (Microns)
Α	.59	3.42
В	.72	3.18
С	.03	5.00*
D	.98	4.83
Ε	.07	3.15

^{*}Defined upper limit

4. INVERSION RESULTS

The data were inverted using the analytic inversion method. 1,2 This method returns only that portion of the solution that depends on the data and the Mie cross section; i.e. it makes no assumptions regarding functional form or smoothness of the size distribution. The inversions were performed in the radius intervals specified in Table 5 and the results plotted in Figures 6 through 10 where the number density for both the lognormal fit and inversion result are shown. Figures 11 through 15 give the corresponding volume density plots where the volume density g is defined as

$$g(r) = \frac{4}{3} \pi r^3 f(r)$$
 (5)

and f(r) is the size distribution obtained through either the log-normal fit or the inversion. However, the following discussion of the inversion results will be based on the number density distribution of Figures 6 through 10.

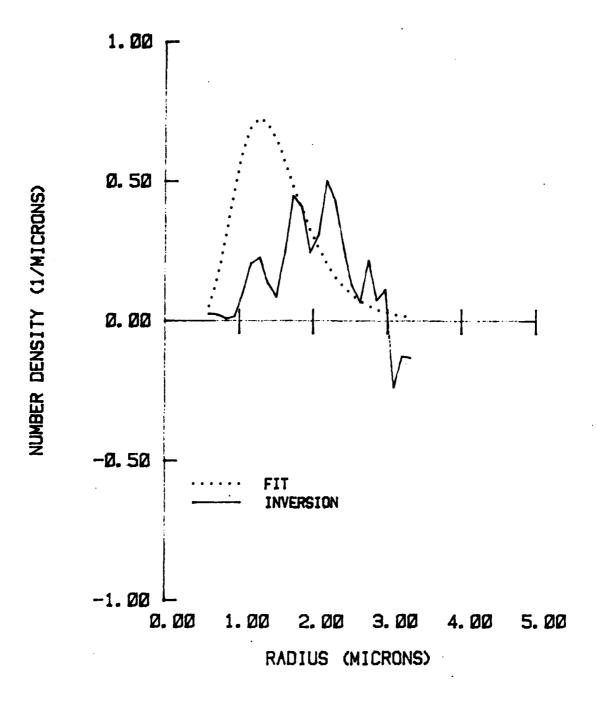


Figure 6. Size Distribution for Set A

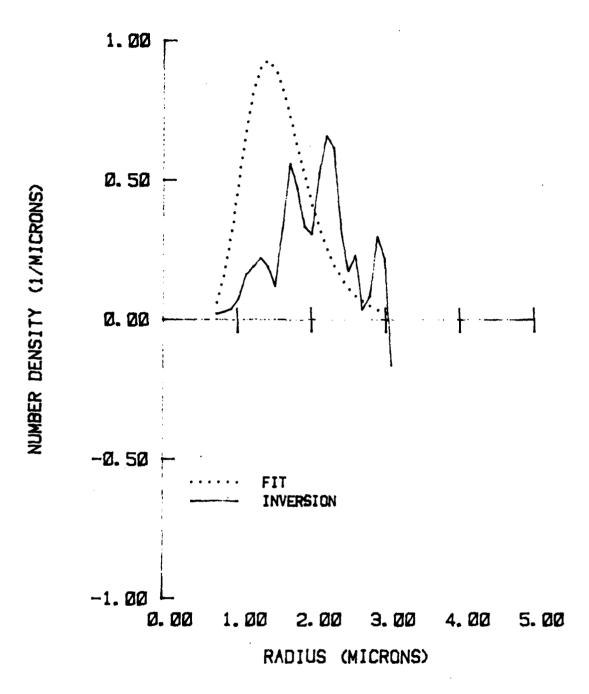


Figure 7. Size Distribution for Set ${\sf B}$

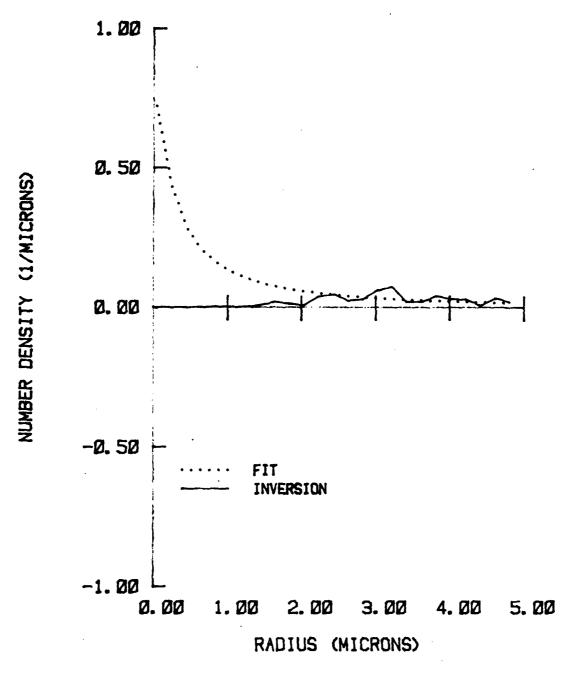


Figure 8. Size Distribution for Set C

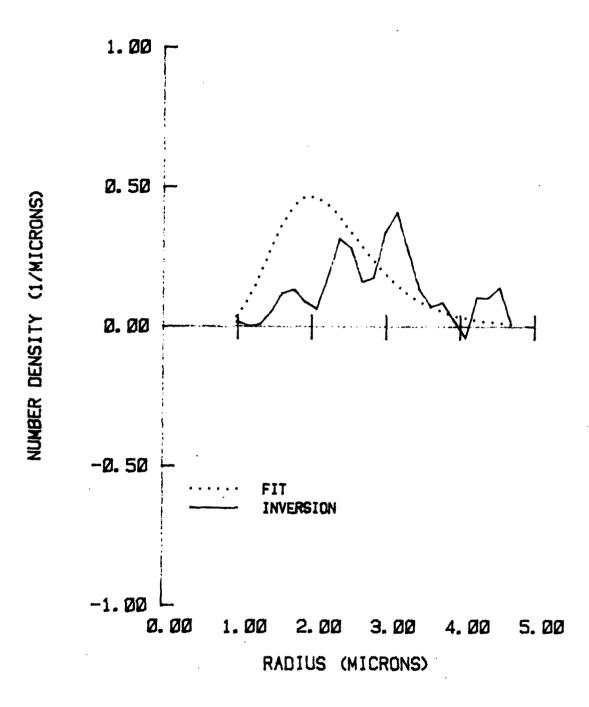


Figure 9. Size Distribution for Set ${\tt D}$

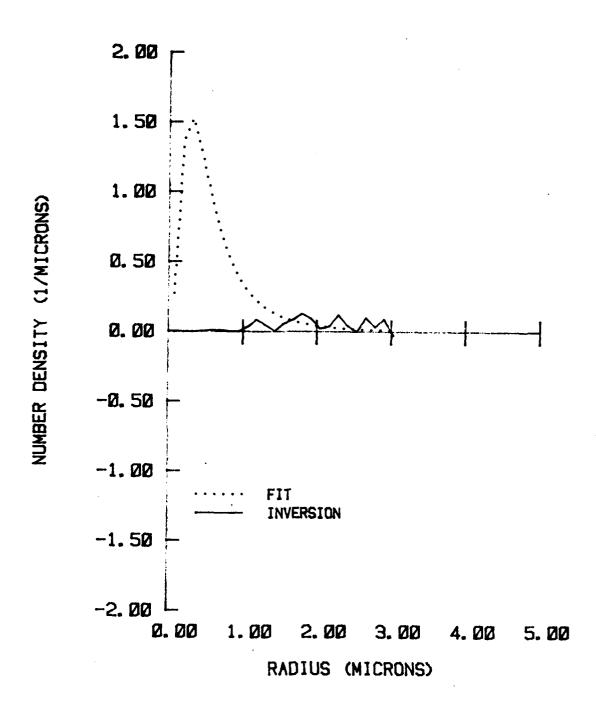


Figure 10. Size Distribution for Set E

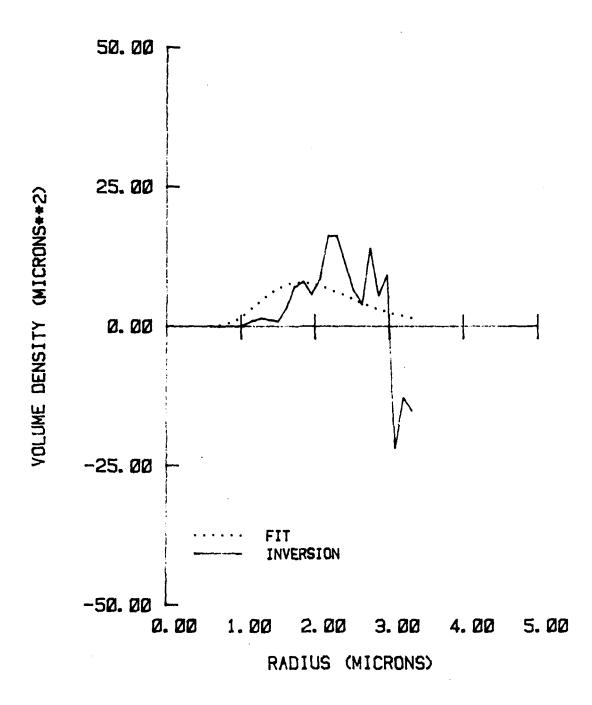


Figure 11. Volume Distribution for Set ${\sf A}$

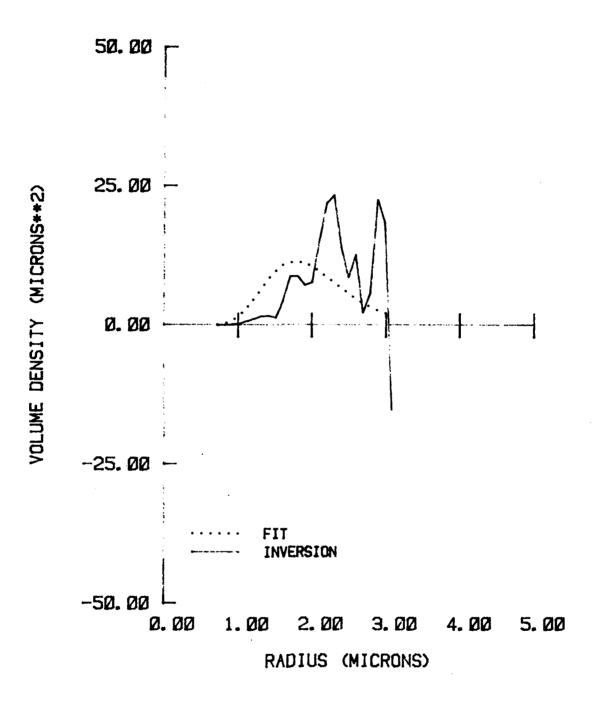


Figure 12. Volume Distribution for Set ${\tt B}$

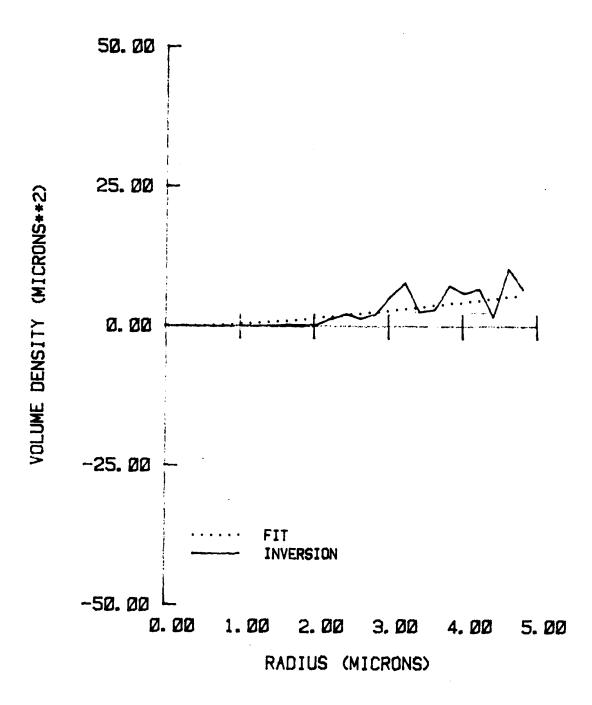


Figure 13. Volume Distribution for Set C

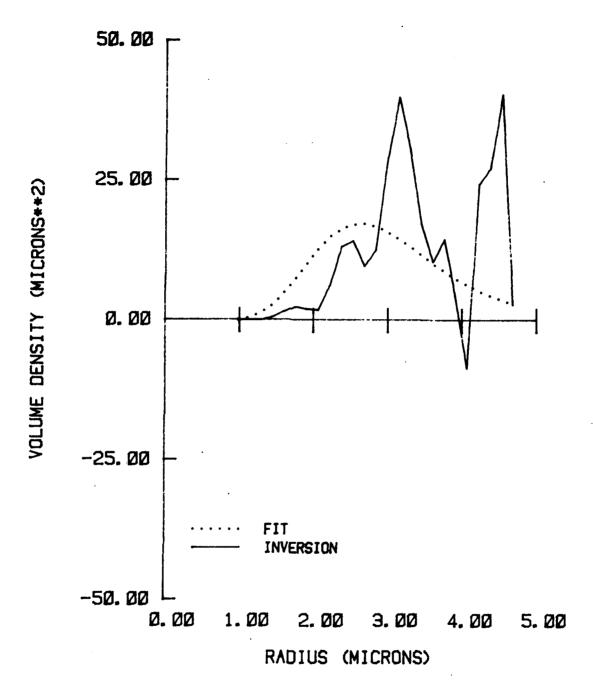


Figure 14. Volume Distribution for Set D

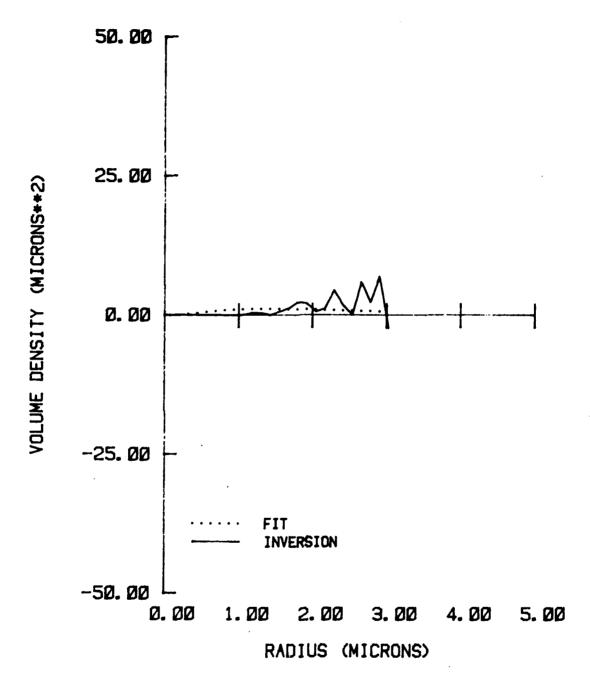


Figure 15. Volume Distribution for Set E

The most consistent feature of the five plots is that the inversion result tends to follow the fit in the upper half of the radius range and tends toward zero in the lower half. This is the expected result, as discussed earlier, since the eigen functions from which the solution must be constructed all tend to zero in this lower radius region. In Sets A, B, and D, where the fit shows significant values in the upper radius region, the inversion is also substantially different from zero and oscillates near the fit value. The size distribution is skewed sharply toward small radius in Sets C and E. In these cases the inversion as well as the fit remains small in the upper radius region.

How much confidence can be placed in the results shown in Figures 6 The chi-square function, Equation 3, may be used to evaluate the goodness of the log-normal fit. Values of chi-square and the associated confidence level, the probability that chi-square has the given or larger value through a random fluctuation, is given in Table 6. If the confidence level is less than 5% the fit is customarily rejected, i.e. the data is not from the distribution tested. By this criterion Sets A, C, D, and E are not drawn from a simple log-normal distribution. interesting to note that the only case for which the fit could not be rejected was Set B which had a larger uncertainty than the others, 10% versus 3%. While the exact form of the distribution is not log-normal the range of sizes should be valid as the fitted distribution and real one must have their major contribution in the same region. Supporting evidence for this comes from the inversion results which make no assumption regarding the form of the distribution. In the upper part of the radius range, the only place the Mie kernels contain reliable information, the fit and inversion results tend to agree.

Table 6. Chi-square Confidence Levels

<u>Set</u>	<u>Chi-Square</u>	<u>Confidence Level</u>
Α	23.6	.03
В	14.3	.3
С	32.1	10 ⁻³ 5 x 10 ⁻⁴
С	34.1	5 x 10 ⁻⁴
E	110	10-8

From results of the direct inversion method it is obvious that the Mie kernels contain little information in the lower half of the radius region. The information contained in the data must be supplemented with assumptions about the function in order to obtain a useful inversion. One approach is to use an inversion method such as constrained linear inversion⁴ which incorporates a smoothing constraint as a basic part of the algorithm. However, this method, along with others, inextricably mixes the effects of the data and constraints. A new method, based on an extension of the analytic inversion technique, which allows introduction of constraints and separates the contributions of the data and constraints is presented in the following section.

5. EXTENSION OF ANALYTIC INVERSION TECHNIQUE TO INCORPORATE CONSTRAINTS

In a previous paper² an analytic inversion technique was developed for Fredholm type remote-sensing problems. A principal result of this work was that only that portion of the solution lying in the space spanned by the kernels could be determined from the data. Often, however, there exists additional knowledge about the solution that could be used. example, if the solution is a particle size distribution then it must be Some other inversion methods, such as constrained linear non-negative. inversion⁴ and the method of Landweber,⁵ make use of a smoothing However, the effects of the data and the constraint are so constraint. entangled that it is not possible to separate their individual influences on the solution. The present work will show how it is possible by using the analytic method and a general assumption about the nature of the solution to apply a constraint to obtain the portion of the solution in the space orthogonal to the space spanned by the kernels. As the two parts of the result (the one determined by the data and the other by the constraint) are independent, their relative contributions can be studied.

The assumption referred to in the preceding paragraph is that the solution function can be expressed to the necessary accuracy by a finite Fourier series. In practice, this is not an unreasonable assumption as the

number of terms may be chosen large enough that a conjectured solution can be represented to a desired accuracy.

We will consider the problem of finding a solution to the system of Fredholm integral equations

$$g_i = \int_{C}^{C+2L} K_i(x) f(x) dx + e_i$$
 $i = 1, 2, N$. (6)

The kernels $K_i(x)$ are known functions representing the physical interaction, the g_i are the experimental measurements, the e_i are random experimental errors, and f(x) is the unknown function, assumed to have a finite Fourier series representation. Results regarding the analytic inversion portion of the problem will be taken from the remote sensing data. 2 The following section will establish terminology and notation.

Let V be the vector space over the reals consisting of continuous, real-valued functions on the interval $C \le x \le C + 2L$ and the inner product on V be

$$<\mathbf{t},\mathbf{u}> = \int_{C}^{C+2L} \mathbf{t}(\mathbf{x}) \ \mathbf{u}(\mathbf{x}) \ d\mathbf{x} \qquad \mathbf{t}, \ \mathbf{u} \in V$$
 (7)

The norm ||u|| of a function u(x) is then

$$||u|| = \langle u, u \rangle^{1/2}$$
 (8)

The finite Fourier series representation of f(x) on the interval C $\leq x \leq C + 2L$ is given by the series

$$f(x) = \frac{c_0}{2} + \sum_{m=1}^{M} \left(c_m \cos \frac{m\pi x}{L} + d_m \sin \frac{m\pi x}{L} \right)$$
 (9)

with unknown coefficients. The kernels $K_{i}(x)$ may be represented on the same interval by the Fourier series

$$K_{i}(x) = \frac{a_{i0}}{2} + \sum_{m=1}^{\infty} \left(a_{im} \cos \frac{m\pi x}{L} + b_{im} \sin \frac{m\pi x}{L} \right)$$
 (10)

where

$$a_{im} = \frac{1}{L} \int_{C}^{C+2L} K_{i}(x) \cos \frac{m\pi x}{L} dx$$
 (11)

$$b_{im} = \frac{1}{L} \int_{C}^{C+2L} K_{i}(x) \sin \frac{m\pi x}{L} dx$$
 (12)

Neglecting for the moment the experimental errors we have from equation (6) by a straightforward calculation.

$$g_i = \langle K_i, f \rangle$$

$$= L \left[\frac{a_{io} c_{o}}{2} + \sum_{m=1}^{M} (a_{im} c_{m} + b_{im} d_{m}) \right]$$
 (13)

Thus, the values g_i are determined only from the Fourier coefficients of the kernels a_{im} and b_{im} with $m \le M$. We will define a set of truncated kernels $K_i^T(x)$ by

$$K_{i}^{T}(x) = \frac{a_{io}}{2} + \sum_{m=1}^{M} \left(a_{im} \cos \frac{m\pi x}{L} + b_{im} \sin \frac{m\pi x}{L} \right)$$
 (14)

where a_{im} and b_{im} are given by equations (11) and (12).

From equation (13) we have

$$g_{i} = \langle K_{i}, f \rangle = \langle K_{i}^{T}, f \rangle$$
 (15)

which can be normalized to give

$$g'_{i} = \langle K'_{i}, f \rangle \text{ and } \langle K'_{i}, K'_{i} \rangle = 1$$
 (16)

where
$$g_i' = g_i/||K_i^T||$$

$$K_{i}^{\dagger}(x) = K_{i}^{\dagger}(x)/||K_{i}^{\dagger}||$$
(17)

$$\mathbf{a}_{im}' = \mathbf{a}_{im}/||\mathbf{K}_{i}^{\mathsf{T}}||$$

$$b_{im}' = b_{im}/||K_i^T||$$

$$||K_{i}^{T}||^{2} = L \frac{a_{io}^{2}}{2} + \sum_{m=1}^{M} (a_{im}^{2} + b_{im}^{2})$$
.

The sine and cosine function appearing in the Fourier series are orthogonal elements of V. It is, therefore, possible to construct a 2M+1 dimensional, orthonormal basis for a subspace V' of V from the functions in the Fourier series of equations (9) and (14). We shall express this basis B in matrix notation.

$$B(x) = \frac{1}{\sqrt{L}} \begin{cases} \frac{1}{2} \\ \cos \frac{m\pi x}{L} \\ \vdots \\ \sin \frac{m\pi x}{L} \\ \sin \frac{m\pi x}{L} \end{cases}$$
(18)

any element u(x) of V' can be expressed as

$$u(x) = U + B(x)$$
(19)

where ${\bf U}$ is a column matrix with 2M+1 real elements and the asterisk denotes matrix transposition. The elements of ${\bf U}$ for a Fourier series expansion, such as equation (9), are given by the relationship

Thus, f(x) and $K_1(x)$ are elements of V'.

Combining equations (13) and (14) we obtain the normal expression for the scalar product of two vectors in an orthonormal basis

$$< t, u > = \sum_{j=1}^{2M+1} t_j u_j$$
 t, $u \in V'$ (21)

If W is the subspace of V' spanned by the $K_i(x)$ and X is the orthogonal complement of W in V', the function f(x) can be written

$$f(x) = r(x) + s(x) \qquad r(x) \in W, \ s(x) \in X. \tag{22}$$

From the definition of the orthogonal complement

$$g_{i}^{'} = \langle K_{i}^{'}, r + s \rangle$$

$$= \langle K_{i}^{'}, r \rangle.$$
(23)

An orthonormal basis $\mathbf{P}(\mathbf{x})$ for W can be constructed from an eigenanalysis of the covariance matrix \mathbf{C} where

$$C_{ij} = \langle K_i, K_j \rangle$$
 (24)

Let p_1 be the eigenvalues of C arranged in decreasing order, i.e., $p_1 \geq p_2 \geq \ldots \geq p_N$, U = matrix whose columns are the unit normalized eigenvectors of C arranged in the same order as the eigenvalues, i.e., column 1 is the eigenvector whose eigenvalue is p_1 , and

If $K^i(x)$ is the column matrix whose elements are the functions $K_1^i(x)$ an orthonormal basis for W is given by

$$P(x) = A U * K'(x)$$
 (26)

The matrix K'(x) can be expressed in terms of the basis B(x) by

$$\mathbf{K}^{\mathsf{T}}(\mathsf{x}) = \mathbf{F}^{\mathsf{T}} \, \mathbf{B}(\mathsf{x}) \tag{27}$$

where F is the (2M+1) x N matrix whose i^{th} column is given in terms of the Fourier expansion coefficients of $K_i(x)$ by equation (20). Equations (26) and (27) lead immediately to the expression of the basis P(x) of V'.

$$P(x) = R B(x) \tag{28}$$

where

$$R = A U^* F^* \tag{29}$$

The solution to equation (23) is

$$r(x) = \mathbf{E}^* \mathbf{P}(x) \tag{30}$$

$$= E*RB(x)$$

where

$$\mathbf{E} = \mathbf{A} \ \mathbf{U}^{+} \ \mathbf{G}^{+} \tag{31}$$

G' being the column matrix whose elements are the g_i^* . The highest index elements of the N x l matrix E may be set equal to zero depending on the uncertainties e_i of equation (6) and the error analysis. 1

Throughout the above derivation it has been assumed that there were N eigenvectors of the covariance matrix C. However, if some of the $K_i(x)$ are linear combinations of the others then there will be N' < N eigenvectors. The above results are valid with the appropriate changes of dimensionality. In the remainder of the paper we shall use N' as the dimension of W to reflect the fact that it may differ from N, the number of equations in (6).

An analytic expression has been given for r(x), that part of the solution f(x) lying in W. However, as seen from equation (23) s(x), the portion of f(x) in the orthogonal space X, is independent of the data. This means that additional information must be applied to the problem in order to determine s(x). Often, other information is available. For example, if f(x) is a probability density function then it must be non-negative.

The first step to finding s(x) is to construct an orthonormal basis Q(x) for X. This can easily be done as the basis B(x) of V' and the basis P(x) of the orthogonal complement of X in V' are known. The dimensionality of Q(x) is M' = (2M+1) - N'.

Let

$$Q(x) = S B(x)$$
(32)

where S is an $M' \times (2M+1)$ coefficient matrix to be determined. The requirement that the spaces W and X be orthogonal complements can be expressed as

$$\langle P_{j}, Q_{j} \rangle = 0$$
 $i = 1, ..., N', j = 1, ..., M'$ (33)

Starting with j = 1 equation (33, provides N' equations of the form

$$\sum_{m=1}^{2M+1} R_{im} S_{1m} = 0$$
 (34)

These may be solved by setting (2M+1) - N' of the S_{1m} equal to an arbitrary constant and solving the N' linear equation for the N' remaining coefficients.

The normalization can then be determined by the requirement $\langle Q_j, Q_j \rangle = 1$. This procedure can be iterated to find the next set of S_{jm} where, in addition to the N' equation of the form of equation (34), there are the j' equations of orthogonality in X

$$\sum_{m=1}^{2M+1} S_{jm} S_{j'm} = 0, j' < j. (35)$$

Thus, the matrix S can be constructed by a well-defined, iterative procedure from R.

The solution f(x) to equation (1) can now be expressed as

$$f(x) = E^* P(x) + H^* Q(x)$$
(36)

where H is the M' x 1 matrix of unknown coefficients to be determined by the constraint. A computationally efficient representation of f(x) is

$$f(x) = (E*R + H*S) B(x).$$
 (37)

The matrix \mathbf{H} may now be determined by applying the constraint to f(x) as all other quantities appearing in equation (37) are known. This would commonly be accomplished by creating an evaluation function from f(x) incorporating the constraint conditions and using a numerical minimizing algorithm to determine the elements of \mathbf{H} .

A convenient measure of the effect of the constraints on the solution is given by the ratio R of the norms of f(x) and s(x).

$$R = \frac{||s||}{||f||} = \left[\sum_{m=1}^{M'} H_m^2\right]^{1/2} \left[\sum_{i=1}^{N'} E_i^2 + \sum_{m=1}^{M'} H_m^2\right]^{-1/2}$$
(38)

The solution f(x) to equation (6) has now been found as the sum of two independent terms, one depending on the data and the other on the constraints. These two, r(x) and s(x), can be studied individually to understand the relative importance of the data and constraints to the solution.

6. RECOMMENDATIONS

The preceeding work shows there are two areas where additional research is needed:

- 1) A wider search should be made for an optimal set of measurements. This search would use a larger number of combinations of wavelengths, angles, and polarization in an attempt to find more than the 12 independent pieces of information that constitute the present optimal set.
- The theory, presented in Section 5, which allows constraints to be added to the analytic inversion technique should be programmed. Different constraints such as requiring a non-negative solution, first or second derivative smoothing, and minimum deviation should be tried and tested against data of the type used in this report.

The research program should provide a better set of experimental measurements to characterize particle size distribution and a better inversion method. This method would contain both the smoothing effects of constraints and the analytic dependence on data and would show the quantitative contributions of each.

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